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**AN ASSESSMENT OF TRANSPORT COEFFICIENT
APPROXIMATIONS USED IN GALACTIC HEAVY ION
SHIELDING CALCULATIONS**

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ABSTRACT

An energy-dependent, perturbation expansion solution for heavy ion transport in one-dimension is used to perform depth-dose calculations for 670 MeV/nucleon ^{20}Ne beams incident upon a thick water target. Comparisons of predictions obtained by using typical energy-independent approximations and those obtained with fully energy-dependent input parameters are made. It is found that the calculated doses are underestimated when the energy-independent input approximations are used. The major source of error, however, is the lack of charge and mass conservation in the Silberberg-Tsao fragmentation parameters.

INTRODUCTION

As the era of the Space Transportation System progresses toward development of a permanent Space Station, manned lunar bases, and possible interplanetary travel, chronic exposures of astronauts and spacecraft to large fluences of galactic heavy ions dictate the need to investigate methods for shielding from these radiations. To properly evaluate passive shield requirements, a comprehensive and accurate theory describing the interaction and propagation of these energetic particles, and their subsequent reaction products, in the spacecraft structure, components, and inhabitants is required. To this end, active research efforts are underway to develop these necessary interaction and transport models.

In previous work, an energy-dependent transport theory capable of describing HZE (high-energy, heavy ion) particle propagation has been developed. Predictions of dose versus depth were made for 670 MeV/nucleon ^{20}Ne beams incident upon a water target and compared with recent experimental measurements (ref. 1). Excellent agreement between theory and experiment was obtained if the input Silberberg-Tsao fragmentation parameters (ref. 2) were renormalized to conserve mass and charge. Without renormalization, predicted doses underestimated the measured values by up to 20 percent in the plateau region (absorber depths less than the Bragg peak location). For depths greater than the Bragg peak location, the predicted doses underestimated the measured ones by nearly a factor of two, even though the transport calculations used fully energy-dependent input parameters. These results are displayed in figure 1.

Since the galactic cosmic ray (GCR) environment is composed of all types of nuclear species covering a very wide energy spectrum, fully energy-dependent transport calculations are impractical because of excessive computer resource requirements. Therefore, simplifications to typical GCR transport calculations (refs. 3 and 4) are made by substituting energy-independent values or expressions for the input parameters. Unfortunately, the

uncertainties introduced into the predictions by these approximations are unclear because the lack of detailed experimental transport data for the GCR environment precludes meaningful comparisons between theory and experiment. Experimental measurements of GCR fluences in the upper atmosphere (ref. 5), taken in the mid-1960's and presented as total fluxes for several groupings of up to ten different nuclear elements each, are based upon a limited number of total events (~6000) with rather large experimental uncertainties (error bars). Although useful for comparison purposes, the cumulative elemental groupings of various nuclei and the associated sizable experimental error bars do not allow meaningful comparisons for radiobiological protection purposes. Alternatively, dosimetric measurements for some LEO (low Earth orbit) missions exist, but unambiguous comparisons (ref. 6) are difficult because of measurement uncertainties and the cumulative effects of uncertainties in the GCR environment, space vehicle mass (shield) distribution assumptions, and the input transport coefficient approximations used in the calculations themselves. Typical differences between theory and experiment are on the order of a factor of two (ref. 6).

In the work reported herein, an assessment of the possible inaccuracies introduced into a heavy ion transport calculation through the use of various input parameter approximations is made by comparing predicted doses for a ^{20}Ne beam incident upon a thick water target with the fully energy-dependent calculations reported previously (ref. 1). In that work, agreement within 5 percent between theoretical predictions and careful laboratory measurements was obtained.

DEPTH-DOSE EXPRESSIONS

In the straight ahead approximation, and neglecting target secondary fragment production, the transport equation is written as

$$\left[\frac{\partial}{\partial x} - \frac{\partial}{\partial E} \tilde{\Sigma}_j(E) + \sigma_j(E) \right] \phi_j(x, E) = \sum_{k>j} m_{jk}(E) \sigma_k(E) \phi_k(x, E) \quad (1)$$

where $\phi_j(x, E)$ is the flux of ions of type j with atomic mass A_j at x moving along the x -axis at energy E in units of MeV/nucleon, $\sigma_j(E)$ is the corresponding macroscopic nuclear absorption cross section, $\tilde{\Sigma}_j(E)$ is the specific stopping power (change in E per unit distance), and $m_{jk}(E)$ is the fragmentation parameter of ion j produced in collision by ion k . In terms of the specific stopping power, the range of the ion is

$$R_j(E) = \int_0^E dE' / \tilde{\Sigma}_j(E') \quad (2)$$

Using an iterative procedure (ref. 1), equation (1) is solved by the method of characteristics. The resultant series solution is used to evaluate the dose as a function of depth

$$D(x) = \sum_j \int_0^\infty dE S_j(E) \phi_j(x, E) \quad (3)$$

for a monoenergetic beam on type M ions of energy E_0 , where the stopping power is

$$S_j = A_j \tilde{S}_j \quad (4)$$

The dose from the radiation field of the primary (incident) beam, obtained by setting the right-hand side of equation (1) equal to zero, is given by

$$D^{(0)}(x) = S_M(E_x) P_M(E_0)/P_M(E_x) \quad (5)$$

where the nuclear attenuation factors are

$$P_M(E) = \exp [-O_M(E) R_M(E)] \quad (6)$$

The average extinction coefficient is defined as

$$O_M(E) = \left[\int_0^E \sigma_M(e) de / \tilde{S}_M(e) \right] / R_M(E) \quad (7)$$

and the residual energy, E_x , is

$$E_x = R_M^{-1} [R_M(E_0) - x] \quad (8)$$

The first perturbation to the homogeneous solution yields the dose contribution from the secondary ions produced by the fragmentation of the

primary beam. This contribution is

$$D^{(1)}(x) \approx \sum_j A_j v_j (E_{u_j} - E_{l_j}) [m_{jM}(E_0) \sigma_M(E_0) P_j(E_0)/P_j(E_{l_j}) - m_{jM}(E_{l_j}) \sigma_M(E_{l_j}) P_M(E_0)/P_M(E_{l_j}) / [\sigma_M(E_0) - \sigma_j(E_0)] x] \quad (9)$$

where the energy spanned by these secondary ions is given by the "lower limit"

$$E_{l_j} = R_j^{-1} \left\{ \frac{v_M}{v_j} [R_M(E_0) - x] \right\} \quad (10)$$

and "upper limit"

$$E_{u_j} = R_j^{-1} \left\{ \frac{v_M}{v_j} R_M(E_0) - x \right\} \quad (11)$$

The range scale parameter, v_j , for the type- j ion is (ref. 1)

$$v_j = Z_j^2 / A_j \quad (12)$$

The second perturbation, which yields the dose contribution from the tertiary ions, is

$$D^{(2)}(x) \approx \sum_{jk} m_{jk} \sigma_k m_{kM} \sigma_M \frac{A_j v_j (E'_{u_j} - E'_{l_j})}{(v_M - v_k)(\sigma_M - \sigma_k)x} \left(\frac{e^{-\sigma_j x} - e^{-\sigma_M x}}{\sigma_M - \sigma_j} - \frac{e^{-\sigma_j x} - e^{-\sigma_k x}}{\sigma_k - \sigma_j} \right) \quad (13)$$

where the energy range spanned by these tertiary ions is given by the "upper limit"

$$E'_{u_j} = R_j^{-1} \left\{ \frac{v_M}{v_j} R_M(E_0) - x \right\} \quad (14)$$

and the corresponding "lower limit"

$$E'_{l_j} = R_j^{-1} \left\{ \frac{v_M}{v_j} [R_M(E_0) - x] \right\} \quad (15)$$

The m and σ terms in equation (13) are evaluated at E_0 . The results of equations (14) and (15) are understood to be zero whenever the right-hand sides are negative. The above expressions can be applied to various shield materials of uniform composition. Each specific application requires knowledge of the appropriate transport coefficients $S_j(E)$, σ_j , and m_{jk} .

TRANSPORT COEFFICIENTS

Stopping Power

The total stopping power is obtained by summing the electronic and nuclear contributions according to the detailed methods given in reference 1.

Nuclear Absorption Cross Section

The macroscopic nuclear absorption cross sections, $\sigma_j(E)$, are determined from the expression

$$\sigma_j(E) = \sum_i \rho_i \sigma_{ij}(E) \quad (16)$$

where the ρ_i are the elemental constituent number densities for the absorber and the $\sigma_{ij}(E)$ are the microscopic nuclear absorption cross sections. The σ_{ij} were taken from reference 7.

Nuclear Fragmentation Parameters

The basic fragmentation parameters, or multiplicities, for projectile nuclei colliding with an absorber are determined from the expression

$$m_{jk}(E) = \frac{\sigma(Z_k, A_k, A_T, Z_j, A_j, E)}{\sigma_k(A_T, E)} \quad (17)$$

where $\sigma(Z_k, A_k, A_T, Z_j, A_j, E)$ is the partial production cross section for a fragment of type A_j and Z_j produced by an ion of type A_k and Z_k colliding with a target of mass A_T and $\sigma_k(A_T, E)$ is the macroscopic absorption cross section for the k th incident ion colliding with the target of mass number A_T . The partial production cross sections are those obtained from the semiempirical formulas of Silberberg and Tsao (ref. 2) augmented by the light fragment production cross sections of Bertini (ref. 8). These have been modified, however, in two ways: (1) rather than scaling by total ion kinetic energy, as suggested in reference 2, the relative target velocity (energy per nucleon) was assumed to be the appropriate parameter for evaluating the hydrogen fragmentation cross sections since particle velocity, rather than total kinetic energy, is approximately conserved in these interactions (ref. 9) and (2) to account for the lack of fragment mass and charge conservation in reference 2, the fragmentation parameters are renormalized to ensure mass and charge conservation. The multiplicative renormalization factor is

$$F = [Z_p A_p / Z_S A_S]^{1/2} \quad (18)$$

where Z_S and A_S are total fragment charge and mass obtained from the formulation of reference 2, and Z_p and A_p are the incident projectile ion charge and mass.

²⁰Ne DEPTH-DOSE RELATIONS

From reference 1, the doses as a function of depth (Bragg curves) for 670 MeV/nucleon ²⁰Ne ions in water, using both the renormalized Silberberg-Tsao fragmentation parameters (VR) and the unrenormalized parameters (ST), are displayed in figure 1 and compared with experimental data obtained at the Lawrence Berkeley Laboratory. Both calculations are fully energy-dependent. Note that the agreement between the theoretical curve labelled VR and the experimental data is excellent. Therefore, for ease of analysis, subsequent calculations for the various input parameter approximations are compared to the VR calculations. Figure 2 displays the ratio of the ST calculation to the VR calculation as a function of depth in the water target. Note that the lack of mass and charge conservation, even though the calculation is fully

energy-dependent, results in significant underestimation of the dose, especially for depths beyond the Bragg peak location (labelled BP).

The typical GCR transport calculation (refs. 3 and 4) utilizes energy-independent absorption cross sections, σ_{ij} , obtained from some form of the Bradt-Peters expression

$$\sigma_{ij} = \pi r_0^2 (A_i^{1/3} + A_j^{1/3} - \delta)^2 \quad (19)$$

where $r_0 \approx 1.26$ fm and $\delta(\sim 0.4)$ is an overlap parameter between the colliding nuclei labelled i and j . Although reasonably accurate at high energies ("asymptotic" region), it is a poor approximation for energies below several hundred MeV per nucleon (ref. 10). To test the sensitivity of the transport predictions to the energy dependence of σ_{ij} , the values were fixed at those for 2 GeV/nucleon incident energies, which are representative of the asymptotic values. The input fragmentation parameters used were the fully energy-dependent ones. Results of the transport calculations are displayed in figure 3. For absorber depths shallower than the Bragg peak location, the doses are underestimated by 15 percent if the Silberberg-Tsao fragmentation parameters (curve labelled VR) are renormalized. If the fragmentation parameters are not renormalized, the dose underestimate increases to ≈ 40 percent (curve labelled ST). For absorber depths beyond the Bragg peak, the underestimates increase to ≈ 20 percent for the VR calculation and ≈ 60 percent for the ST calculation. Although not displayed in the figures, comparable results are obtained if the absorption cross sections are fixed at the values for 670 MeV/nucleon rather than the "asymptotic" values.

In addition to the use of energy-independent input absorption cross sections, the use of energy-independent fragmentation parameters is an additional possible simplification to the heavy ion transport problem. To test this assumption, transport calculations for the neon beam in water were performed using fragmentation parameters, m_{jk} , fixed at the values applicable to the incident energy of 670 MeV/nucleon and with the absorption cross sections also fixed at their "asymptotic" values. The results, displayed in figure 4, consist of ratios of calculated doses with the input parameters fixed to the doses for the fully energy-dependent calculations. As before, VR labels the calculation using renormalized fragmentation parameters, and ST labels the unrenormalized predictions. Surprisingly, a slight increase in the dose ratios is observed, beyond the Bragg peak, when compared to the predictions obtained for the cases where only the absorption cross sections were fixed (fig. 3). For the VR calculations, the dose underestimates range up to 20 percent for depths shallower than the Bragg peak location and quickly return to less than 10 percent for depths deeper than the Bragg peak. For the ST calculations the dose underestimates are 40 percent and 60 percent, respectively, for depths shallower and deeper than the Bragg peak. To investigate the reason for this improved agreement between the energy-dependent and energy-independent calculations when m_{jk} were fixed, the

transport calculations were repeated for the case where the m_{jk} were fixed and the σ_{ij} were allowed to take on their fully energy-dependent values. The results are plotted in figure 5. For the VR calculations, the sole use of 670 MeV/nucleon fragmentation parameters has almost no effect on the predicted doses for depths shallower than the Bragg peak. For depths beyond the Bragg peak the doses are overestimated by 10-20 percent. Therefore, the use of energy-independent fragmentation parameters partially compensates, at depths greater than the Bragg peak, for dose underestimates resulting from the use of energy-independent absorption cross sections. For the ST calculations, similar trends are observed although the lack of fragment mass and charge conservation results in calculated doses which remain severely underestimated.

SUMMARY

In summary, the use of energy-independent transport coefficients for neon beams in water results in dose underestimates when compared to a fully energy-dependent dose calculation. When coupled with the use of Silberberg-Tsao fragmentation parameters, which are not renormalized so as to conserve fragment mass and charge, the dose is underestimated by up to 40 percent at depths shallower than the Bragg peak. For depths greater than the Bragg peak, the dose is underestimated by up to a factor of 3.

SYMBOLS

A_j	atomic mass of type-j ion, amu
A_T	mass number, dimensionless
$D(x)$	energy absorbed per unit mass at x , MeV/g
E	ion kinetic energy, MeV/amu
E_x	residual energy, MeV/amu
E_0	incident beam energy, MeV/amu
j	type-j ion
k	type-k ion
$m_{jk}(E)$	multiplicity of type-j ions produced by collisions of type-k ions of energy E
$O_M(E)$	average extinction coefficient for type-M ions, cm^{-1}
$P_M(E)$	nuclear attenuation factor for type-M ion at energy E , dimensionless

$R_j(E)$	continuous slowing-down range of type-j ion of energy E , cm
$R_j^{-1}[R_j(E)]$	inverse function of $R_j(E)$
$S_j(E)$	total stopping power or linear energy transfer (LET) due to interaction of type-j ion with orbital electrons of transport medium, MeV/cm
$\bar{S}_j(E)$	stopping power or linear energy transfer (LET) per nucleon due to interaction of type-j ion with orbital electrons of transport medium, MeV/amu-cm
x	one-dimensional position vector, g/cm ²
Z_j	atomic number of type-j ion
v_j	range scale parameter for type-j ion
ρ_i	number density of i th constituent of absorber, cm ⁻³
$\sigma_j(E)$	macroscopic absorption cross section for type-j ion of energy E , cm ⁻¹
$\sigma_{ij}(E)$	microscopic absorption cross section for type-j particle of energy E colliding with type- i particle in absorber, cm ²
$\phi_j(x,E)$	differential flux of type-j ions at x with energy E , (cm ² -sec-MeV/amu) ⁻¹

Subscripts:

M	type of ions in monoenergetic beam
P	projectile
S	Silberberg-Tsao formalism

Superscripts:

(0),(1),(2) terms in series approximation to equation (3)

Primes indicate a variable of summation or integration.

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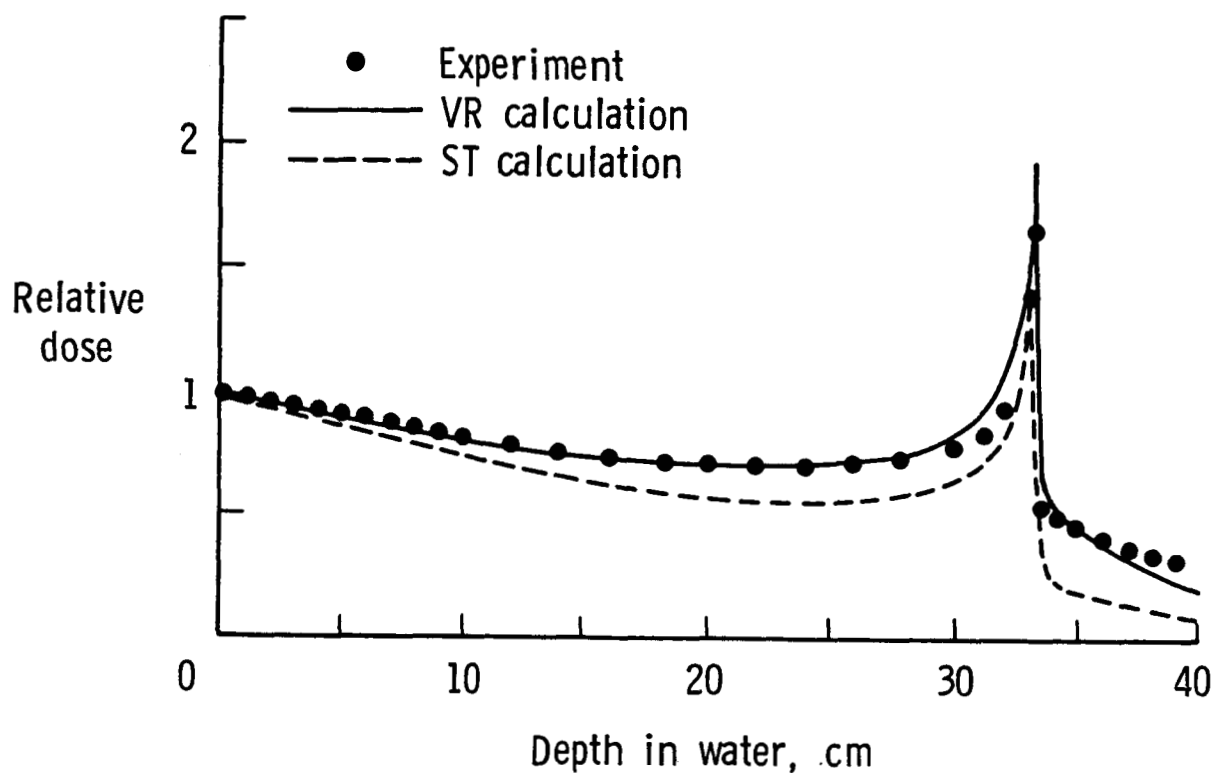


Figure 1.- Energy deposition in water by 670 MeV/nucleon ^{20}Ne ions calculated using Silberberg-Tsao (ST) and renormalized (VR) fragmentation parameters. The experimental results are from Lawrence Berkeley Laboratory. The dose relative to zero absorber thickness is displayed on the ordinate. Both calculations are fully energy-dependent.

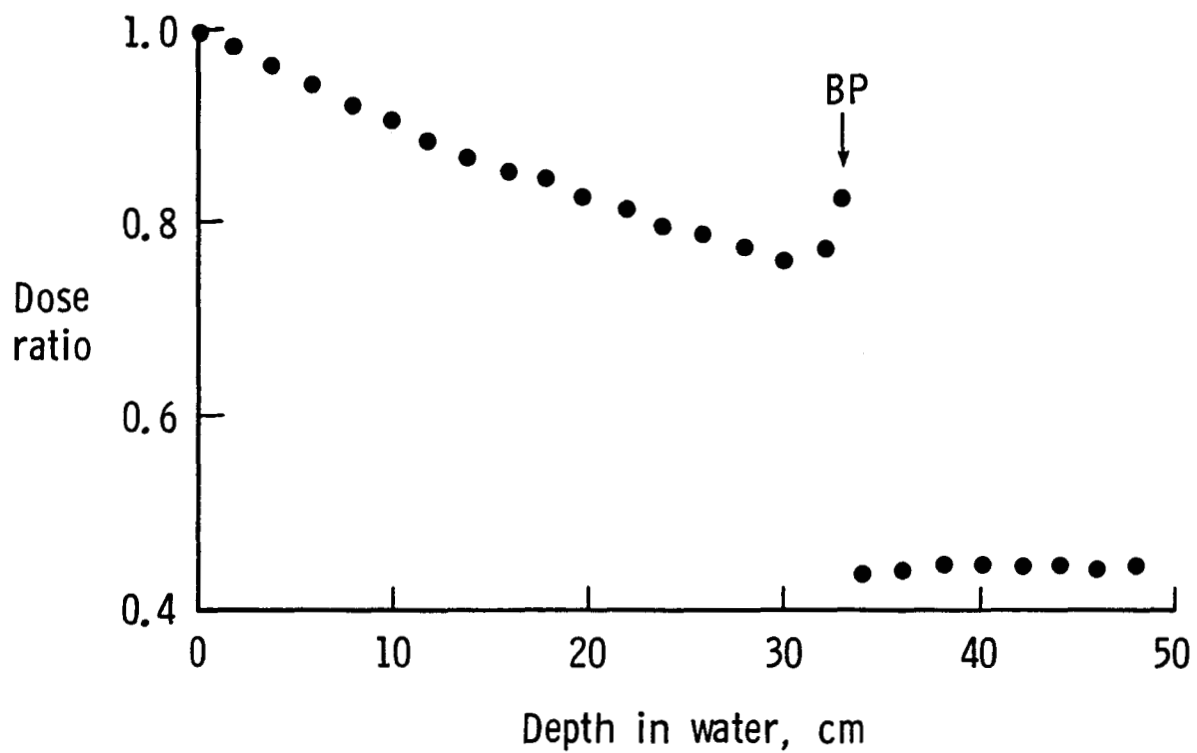


Figure 2.- Ratio of the dose for the ST calculation to the dose for the VR calculation as a function of depth in water. The Bragg peak location is labelled BP for reference.

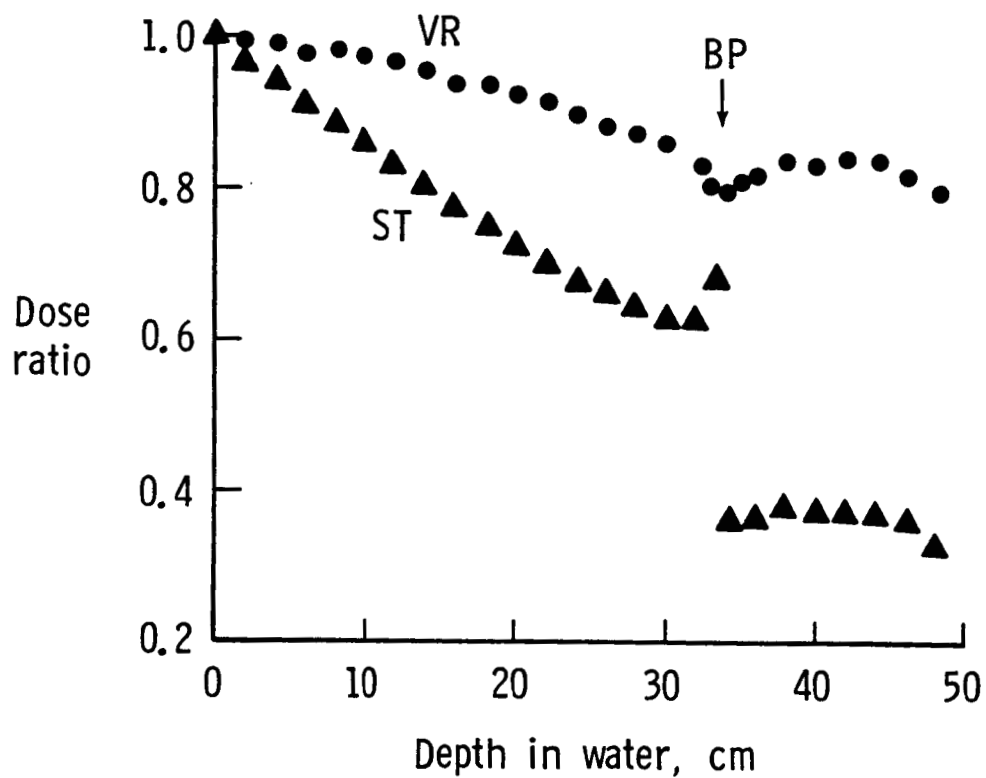


Figure 3.- Ratio of the dose calculated with energy-independent absorption cross sections to the dose calculated with the full energy dependence. Calculations using Silberberg-Tsao (ST) and renormalized (VR) fragmentation parameters are displayed. BP denotes the Bragg peak location.

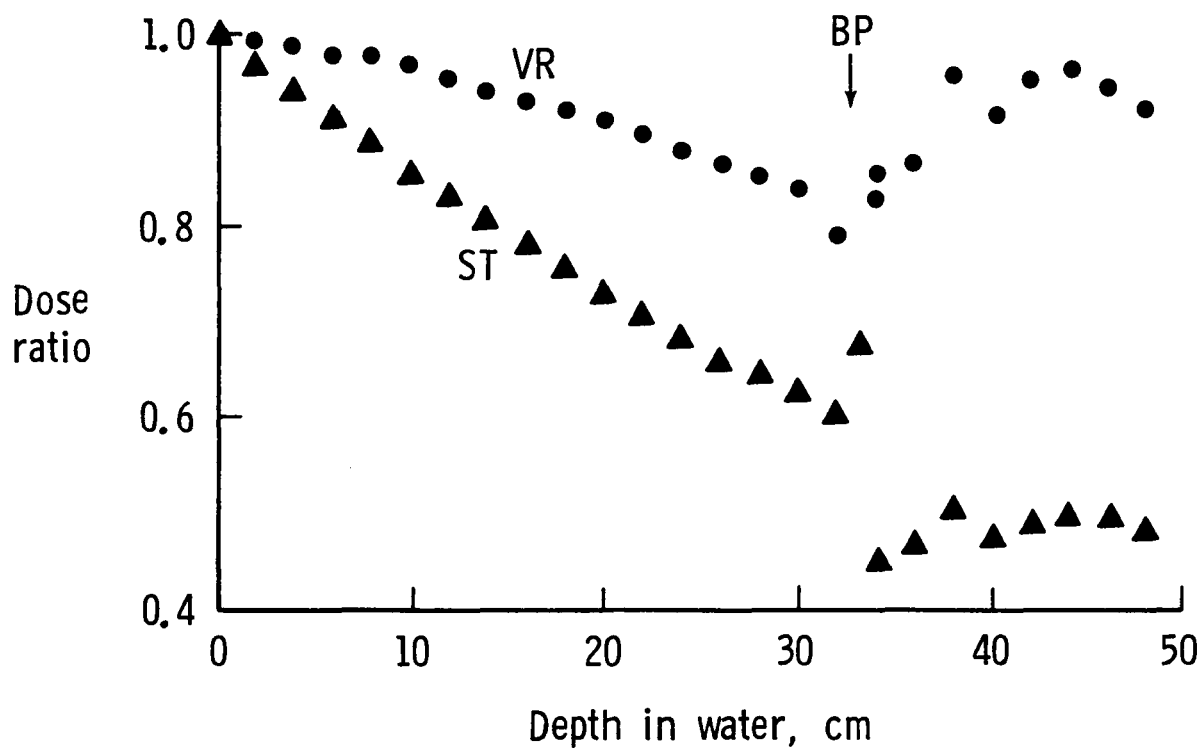


Figure 4.- Ratio of dose calculated with energy-independent absorption and fragmentation cross sections to the dose calculated with the full energy dependence. Calculations using Silberberg-Tsao (ST) and renormalized (VR) fragmentation parameters are displayed. BP denotes the Bragg peak location.

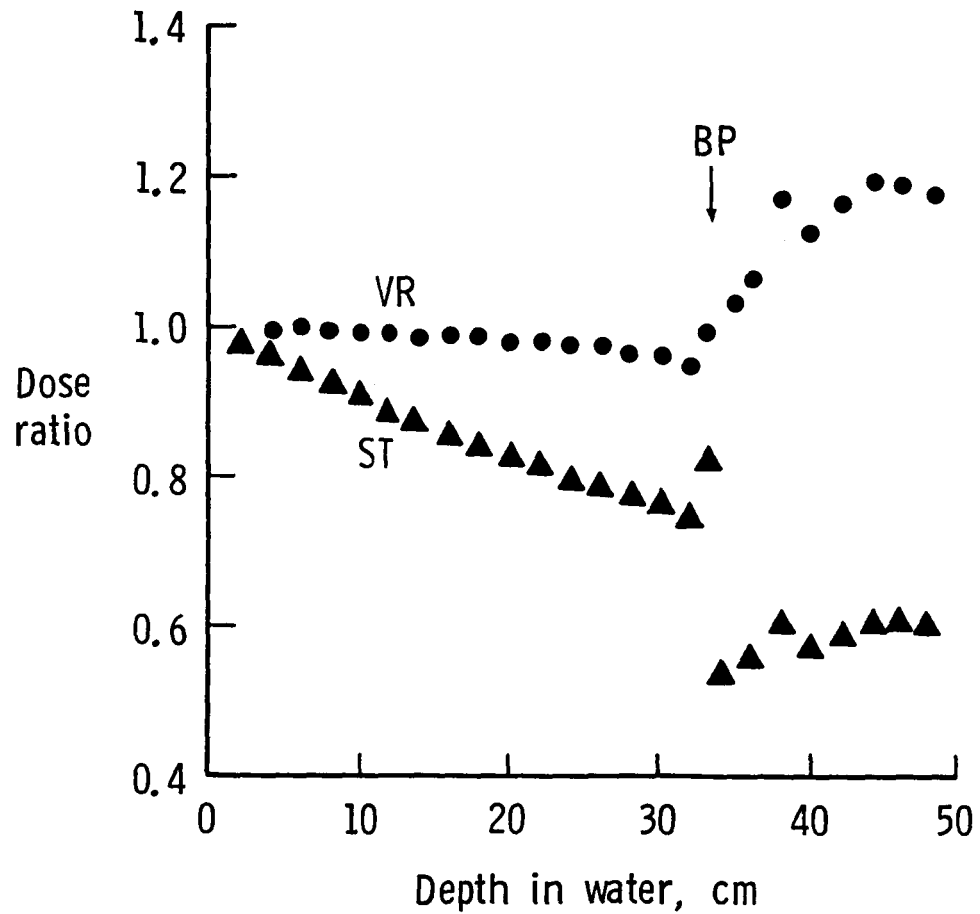


Figure 5.- Ratio of dose calculated using energy-independent fragmentation cross sections to the dose calculated using the full energy dependence. Calculations using Silberberg-Tsao (ST) and renormalized (VR) fragmentation parameters are displayed. BP denotes the Bragg peak location.

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